Tetrahydrophthalic anhydride 85-43-8 | DTXSID3026516

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.25

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 6.37e-01

Nearest Neighbors from the Training Set

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2-Isopropyl-6-methyl-4-

pyrimidone Measured: 1.82 Predicted: 2.23

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4-Methylimidazolidine-2-thione

Measured: 10.0 Predicted: 4.59

Image not found

1,4-Dioxane

Measured: 5.01e-01 Predicted: 1.06

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4-IsobutyImorpholine

Measured: 1.78

Predicted: 2.69

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Paraldehyde Measured: 3.02 Predicted: 2.77